



Phenolic Resin Thermal Response and Fracture in a Bonded-Particle Model

Andrew P. Santos, Lauren J. Abbott, Justin B. Haskins

Thermal Protection Materials Branch NASA Ames Research Center, Moffett Field, CA, USA



August 6, 2025

Thermal & Fluids Analysis Workshop (TFAWS) 2025

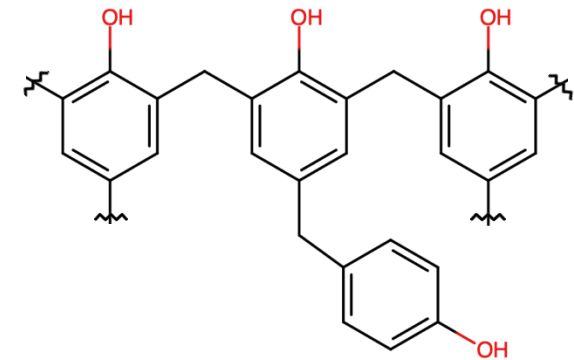
Phenolic-Containing Thermal Protection Materials



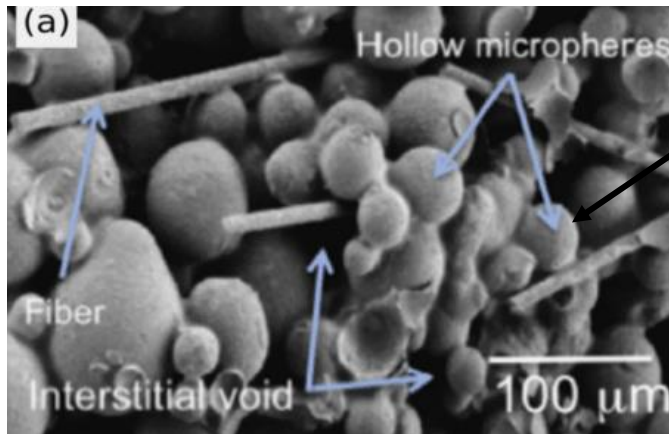
Phenolic resin provides excellent ablative properties at a low density

Support structure:

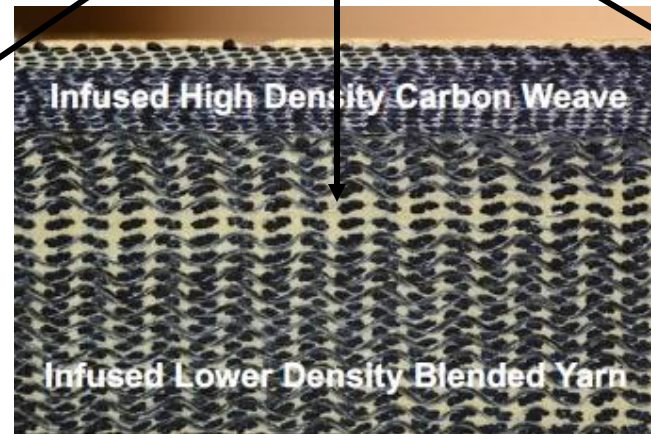
- Glass fiber (AVCOAT),
- Carbon fiber network (PICA)
- Carbon fiber weave (3MDCP, HEEET)



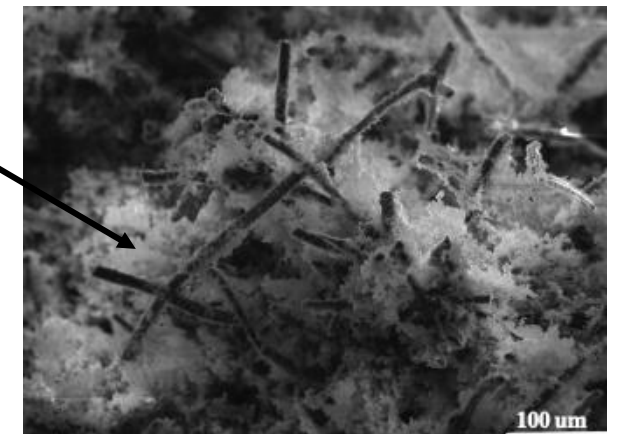
Phenolic resin



Phenolic hollow spheres, fiberglass, epoxy, (Avcoat)



3D woven carbon-phenolic blended yarns infused with phenolic resin



Phenolic Impregnated Carbon Ablator

Sawant, S. et al. *IJHMT* **2019**, 133, 1176–1195.

D Ellerby et al, *MS&T*, 2019; Bessire, B. et al. *ACS Appl. Mater. Interfaces* **2017**, 9 (25), 21422–21437

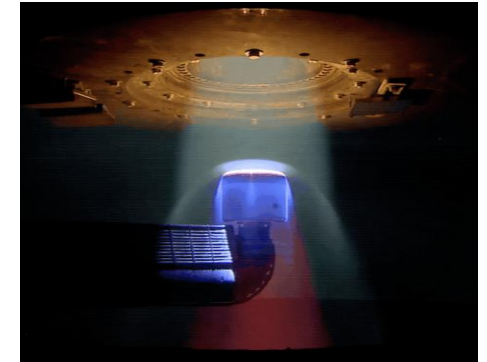
Agrawal, Chavez-Garcia, *J. Spacecraft Rockets*, (4) 50, 2013

Thermal Response of Phenolic-Containing Materials



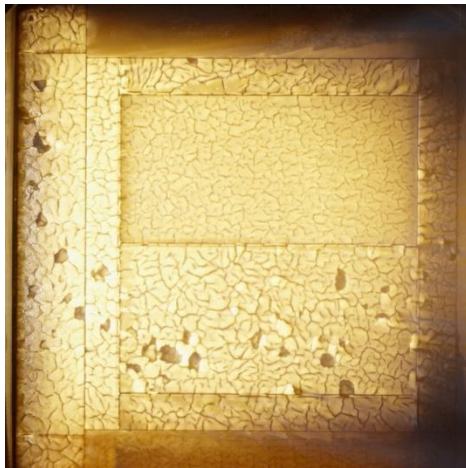
Phenomena we want to capture:

- Entry
- How does fracture affect entry, from
 - MMODs, manufacturing, entry stresses

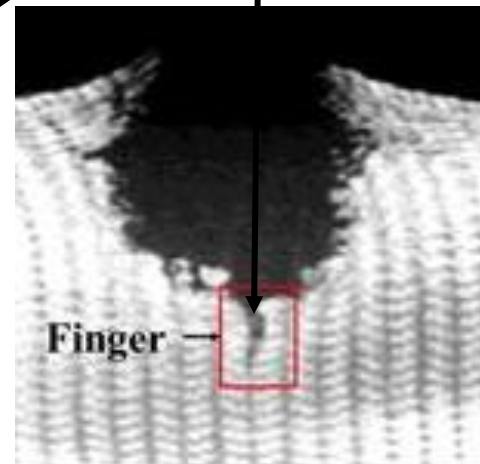


PICA ablating in the ArcJet. NASA

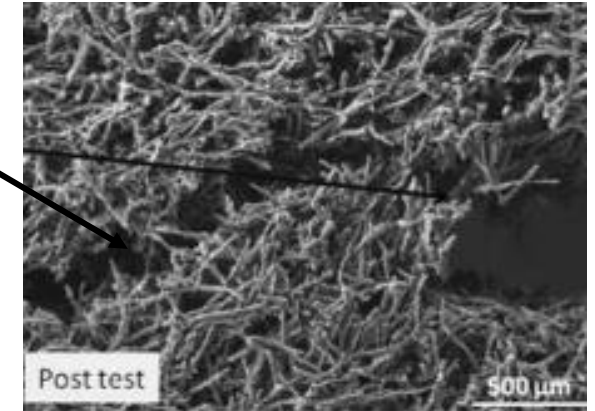
Phenolic drives fracture



Avcoat fracture in ArcJet. NASA

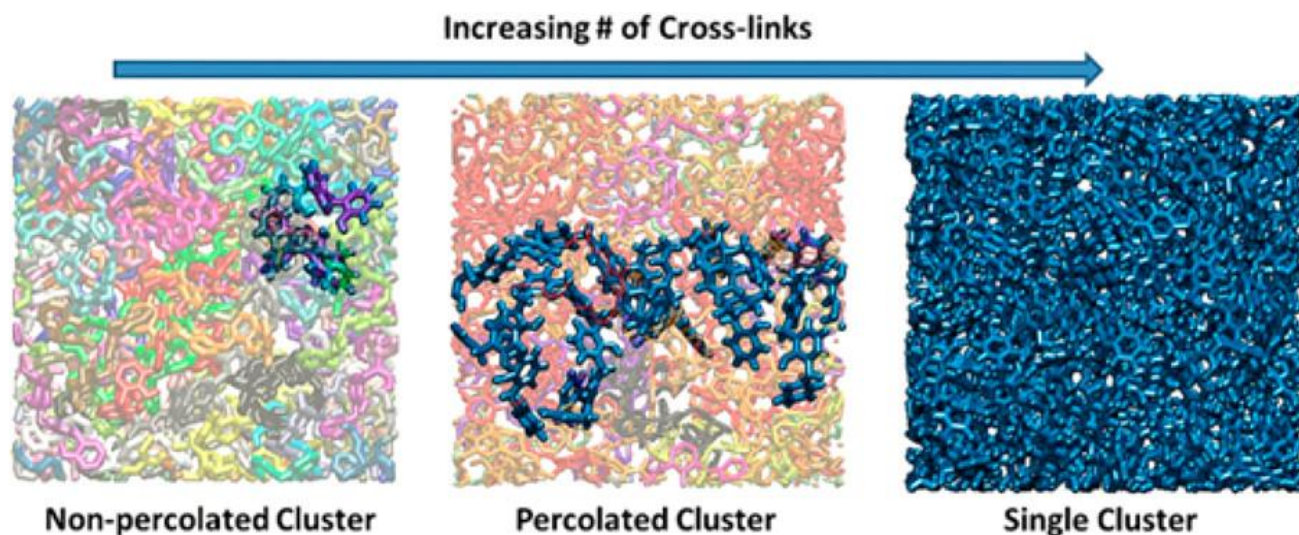


Impact of a woven TPS



SEM of fractured PICA

Computational Approaches to Phenolic models

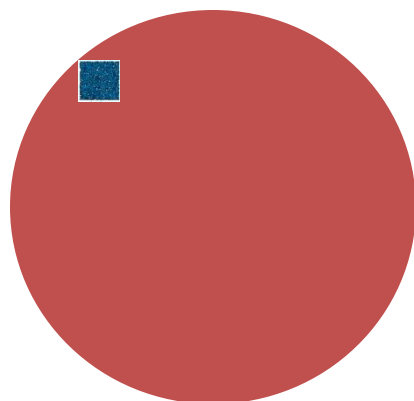


Molecular dynamics

- Simulate each atom with classical statistical mechanics
- bridge RXN competition
- Role of crosslinking on conductivity, modulus, CTE
- Cross link density effect on fracture behavior

Bonded particle

- Between statistical and continuum mechanics
- 10^4 - 10^{10} monomers/particle
- Bond modes of deformation follow experimental parameterization



Abbott, A. et al. ACS Fall 2022

Monk, J. D. et al. *Polymer* **2015**, 62, 39–49.

Monk, J. D.; et al. *Macromol.* **2015**, 48 (20), 7670–7680.

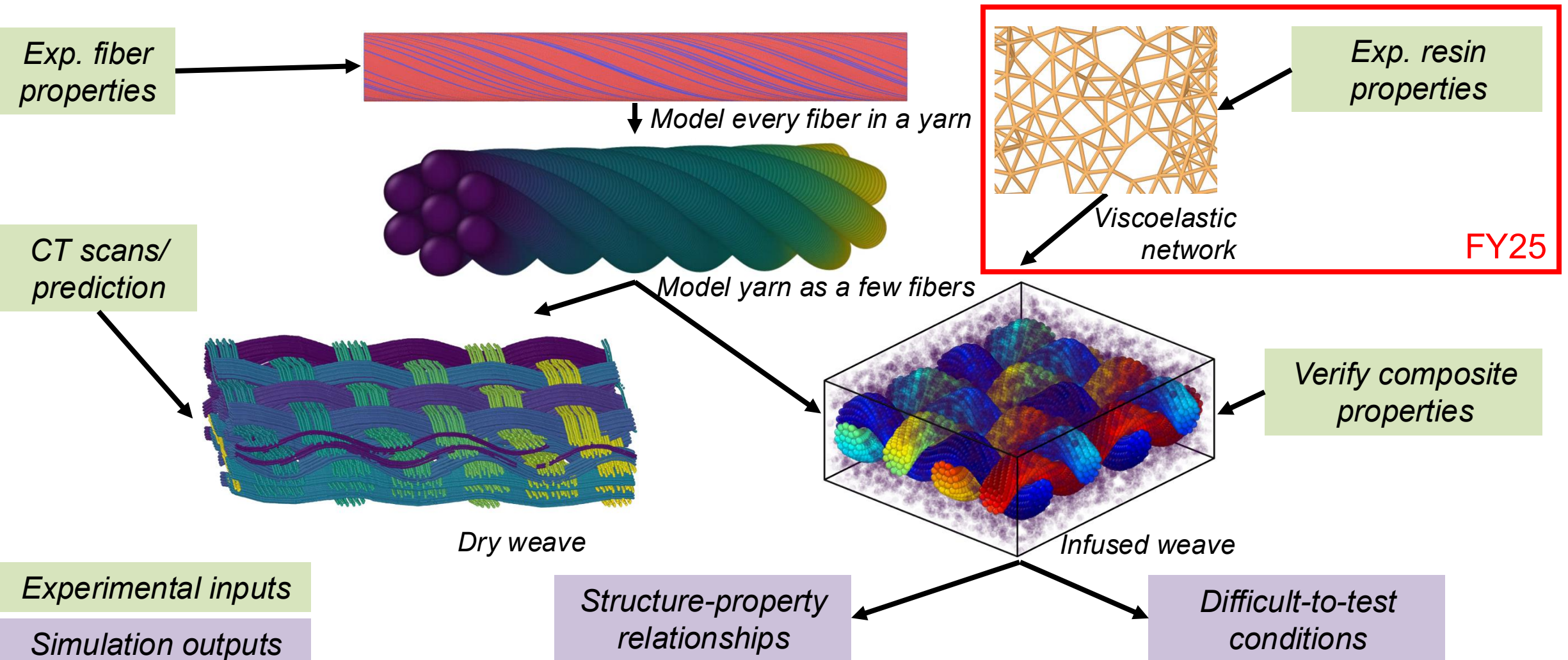
Santos, et al. *Particles*, 2023

Bonded Particle Models for Composites



Long term goal:

Simulate TPS under difficult-to-test conditions with constituent properties

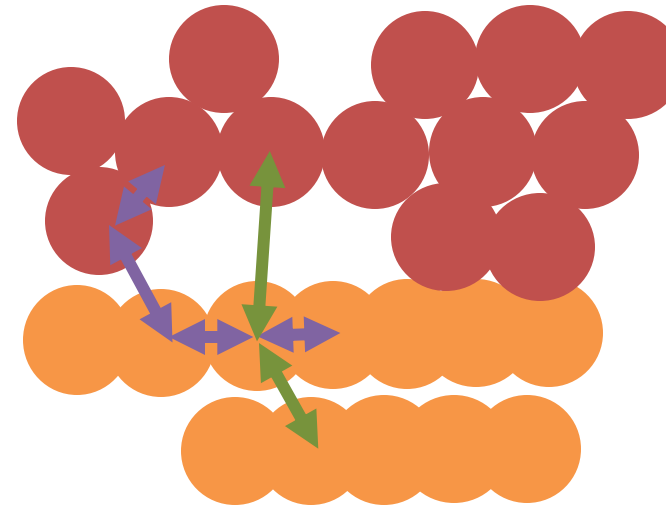


Bonded Particle Model Parameters



Micromechanics-informed model:

- Intra-fiber, fiber-resin, resin-resin^{1,2}, bonded forces
 - Elastic stretch, bend, shear, twist
 - Viscous damping
 - Rupture
- Inter³-fiber and fiber-(void)-resin, contact forces
 - Friction
 - Viscoelastic repulsion
 - Cohesion



- Resin scale matched to fiber: 10^4 - 10^{10} monomers/particle
- Fiber-to-particle ratio:
 - refined fiber=0.1
 - fiber=1
 - Yarn=1000

Component	Input Property
Resin	porosity, $\tan\delta$
Fibers	density, diameter, friction, contact modulus
Resin, fibers, resin-fiber bonds	conductivity, heat capacity tensile, shear, flexural moduli & strength,

¹Chen, X. et al. Comparative Assessment and Unification of Bond Models in DEM Simulations. *Granular Matter* **2021**, 24 (1), 29.

²Wang, Y. and Sun, X. Digital-Element Simulation of Textile Processes. *Composites Sci. Tech.* **2001**, 61 (2), 311–319.

³Silbert, L. E. et al., Granular Flow down an Inclined Plane: Bagnold Scaling and Rheology. *Phys. Rev. E* **2001**, 64 (5), 051302.

⁴Plimpton, S. J. et al., LAMMPS *Comp. Phys. Comm.* **2022**, 271, 108171]

Resin Configuratoin Generation

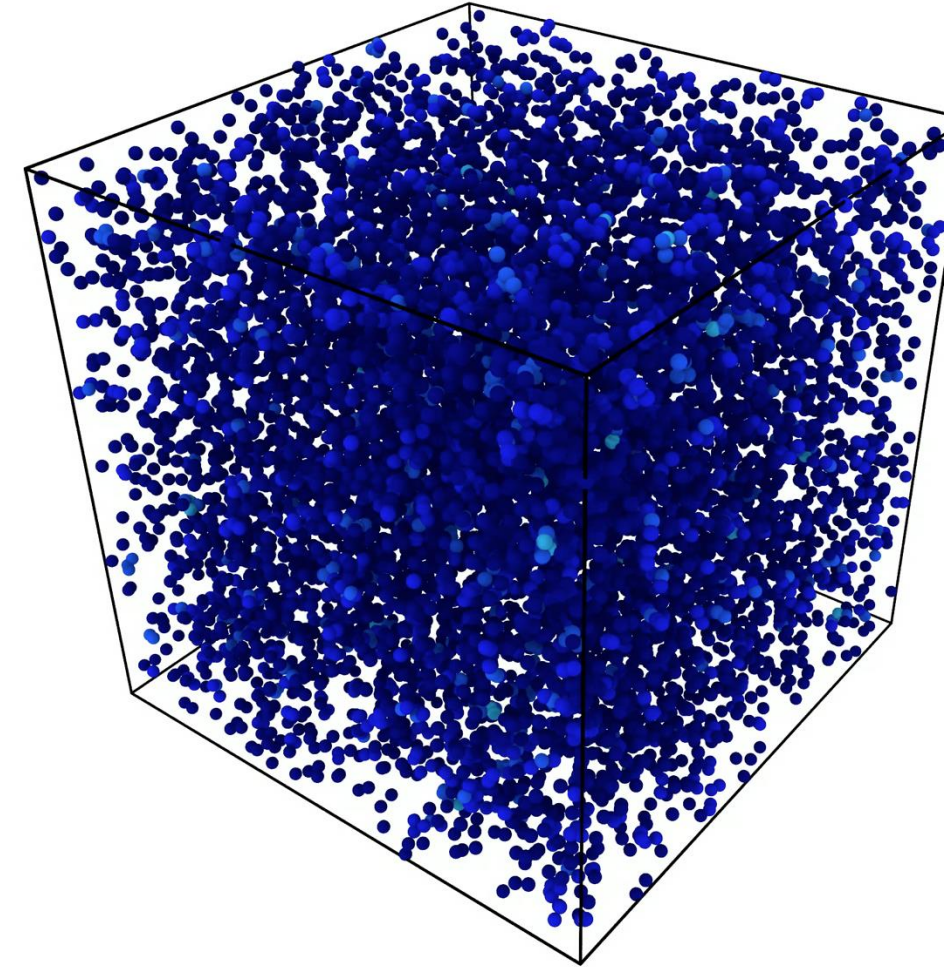


1. Generate random packing:

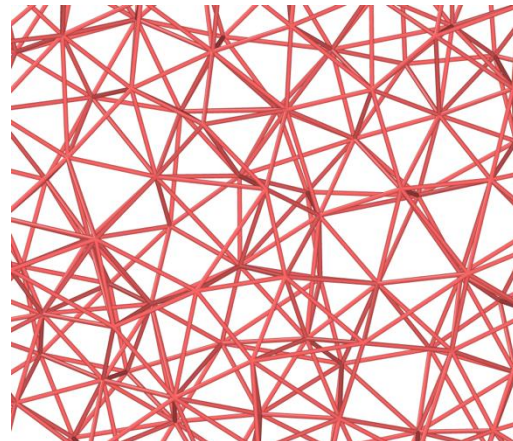
- 20,000 particles in Start from a low volume fraction
- Vary triclinic box dimensions to satisfy a very low pressure tensor
- Discrete element modeling (DEM) with frictionless Hertzian contacts

2. Add bonds:

- contacting and next-nearest neighbors (within $\sim 1.5D$); 10-17 bonds/particle
- Vary bonding radius $R_b=7.5, 8.5\mu\text{m}$ ($\langle N_{\text{bonds}} \rangle=11, 13.4$ respectively)



Granular packing to form random network



Visualization of a slice of the bond network.

Plimpton S. (1995). *J. Comput. Phys.*, 117, 1-19.
Mindlin, R. D. (1949). *J. Appl. Mech., ASME* 16, 259-268.
Luding, S. (2008). *Granular matter*, 10(4), 235.
Santos, A.P. et al. (2020). *Phys. Rev. E*, 102 (3), 032903
CIF22, ESPUR
Clemmer, J. T. et al. (2022) *Phys. Rev. Lett*, 129 (7), 078002

Explicit Porosity and Network Connectivity



1. Generate random packing:

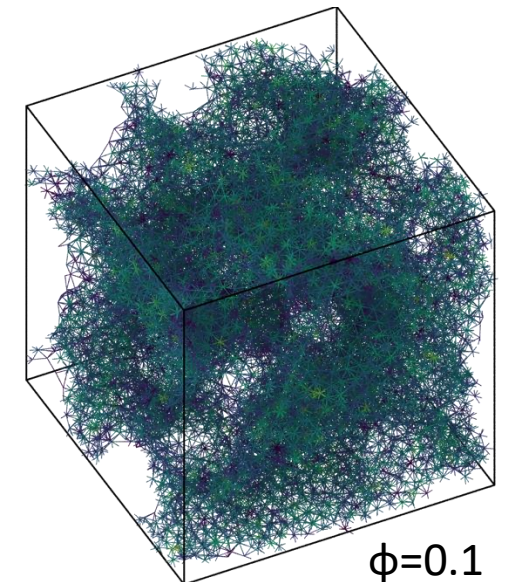
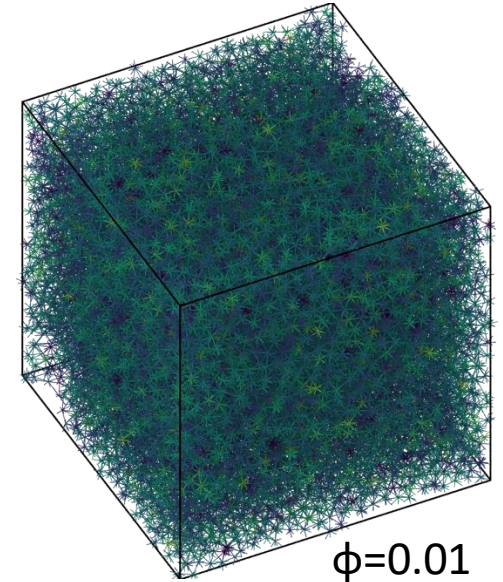
- 20,000 particles in Start from a low volume fraction
- Vary triclinic box dimensions to satisfy a very low pressure tensor
- Discrete element modeling (DEM) with frictionless Hertzian contacts

2. Add bonds:

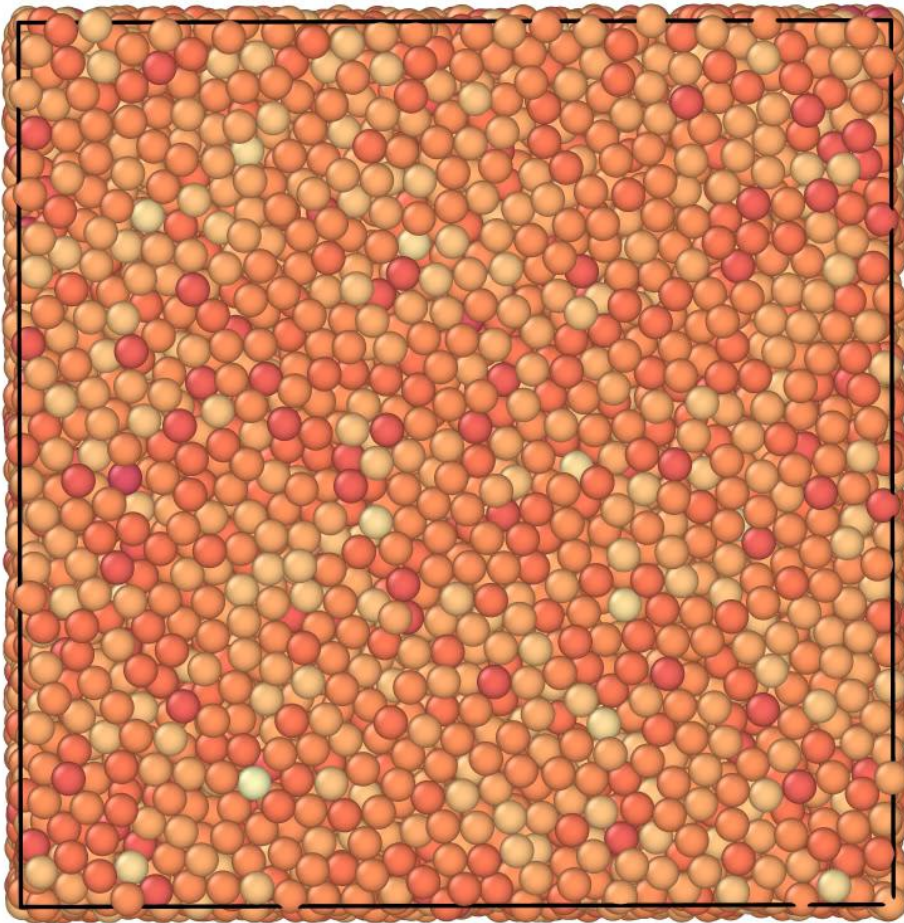
- contacting and next-nearest neighbors (within $\sim 1.5D$); 10-17 bonds/particle
- Vary bonding radius $R_b=7.5, 8.5\mu\text{m}$ ($\langle N_{\text{bonds}} \rangle=11, 13.4$ respectively)

3. Add Porosity explicitly

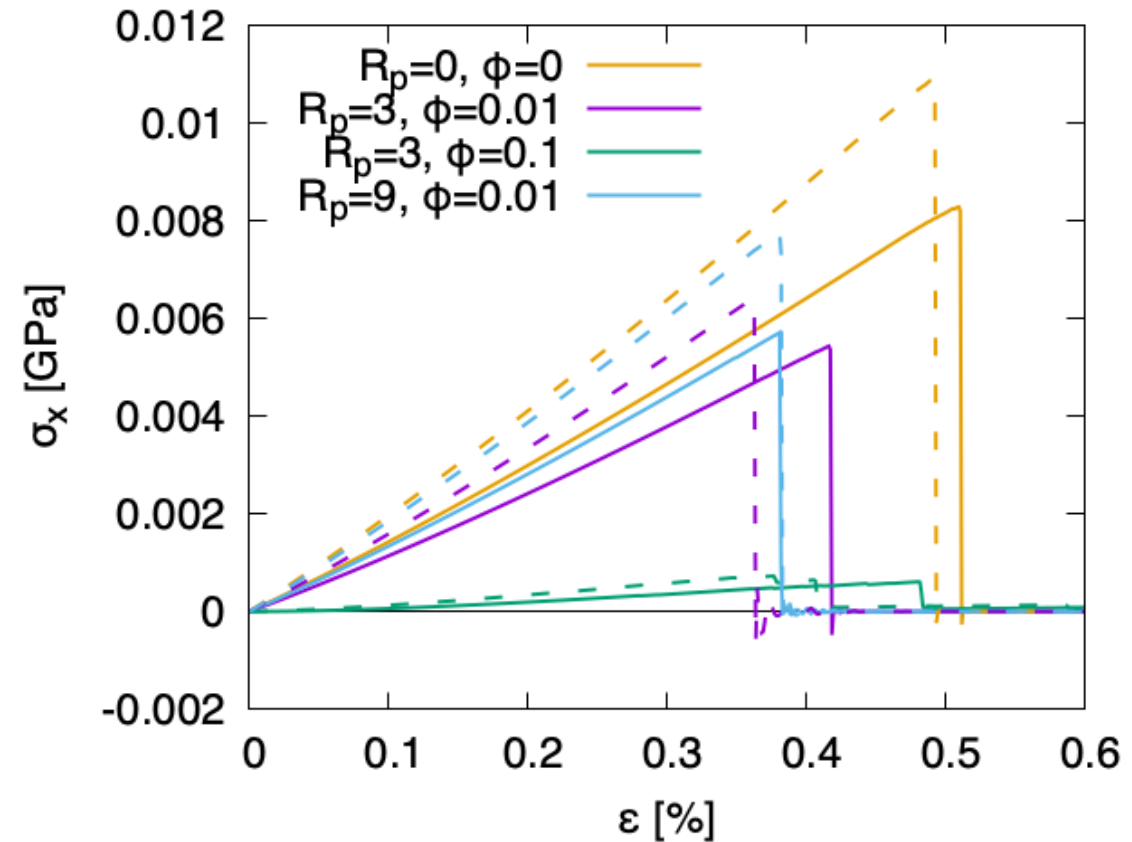
- Delete spherical segments of material
- Vary pore radius $R_p=3\mu\text{m}, 9\mu\text{m}$ (0.5D and 1.5D)
- Vary porosity $\phi=0.01, 0.1$



Tensile Deformation

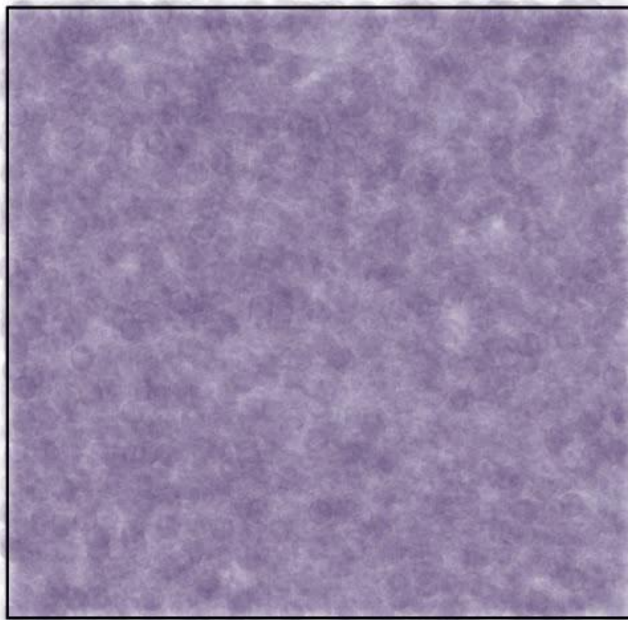


Phenolic resin bonded particle model tensile simulation, particles are colored by number of bonds (black:0 to orange:17)

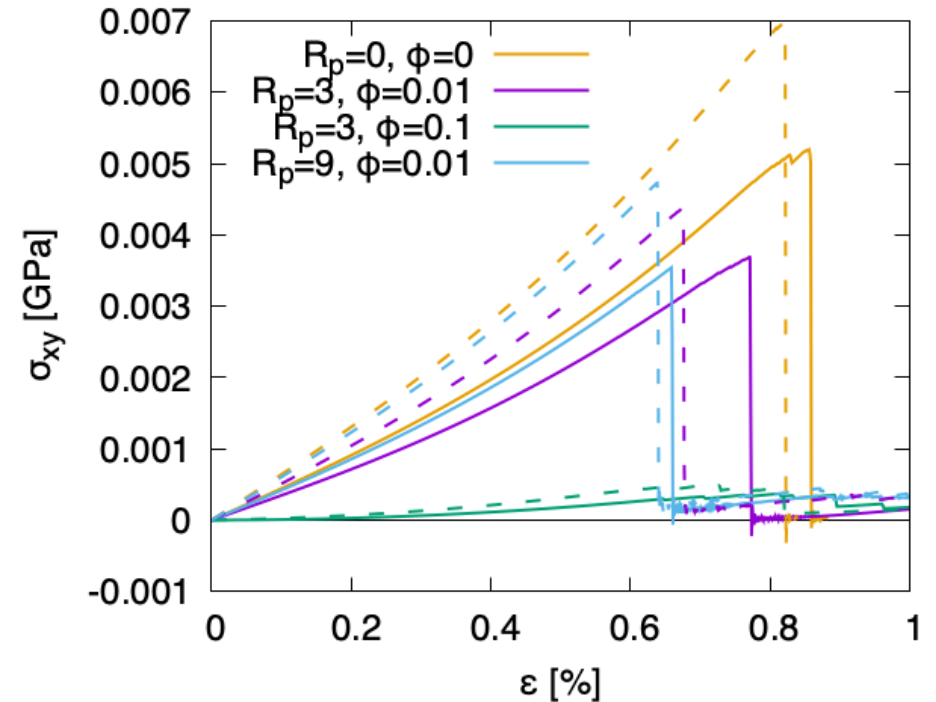


Preliminary tensile stress vs strain $\langle N_{\text{bonds}} \rangle = 11$ (solid) and 13.4 (dashed), and porosity features.

Shear Deformation

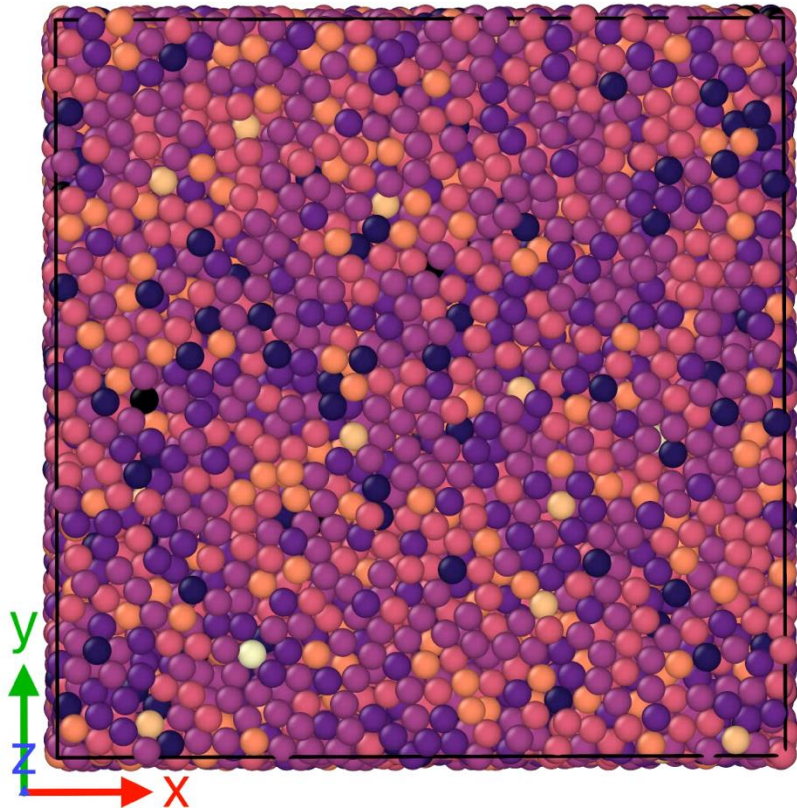


Phenolic resin bonded particle model shear simulation. Particles are colored by per-particle stress (black:-0.25 to orange:2.85 GPa. Transparency increases with number of bonds (max 17, min 0).

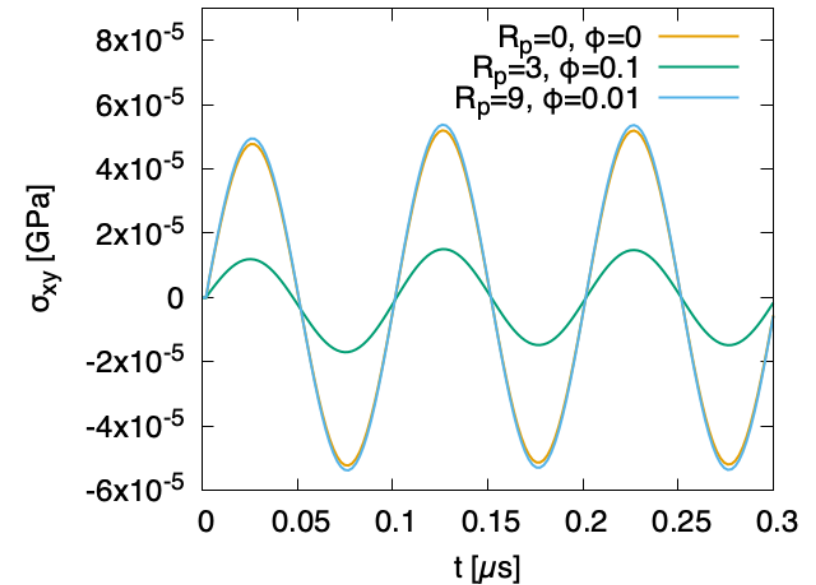


Preliminary shear stress vs strain $\langle N_{\text{bonds}} \rangle = 11$ (solid) and 13.4 (dashed), and porosity features.

Storage and Loss Modulus

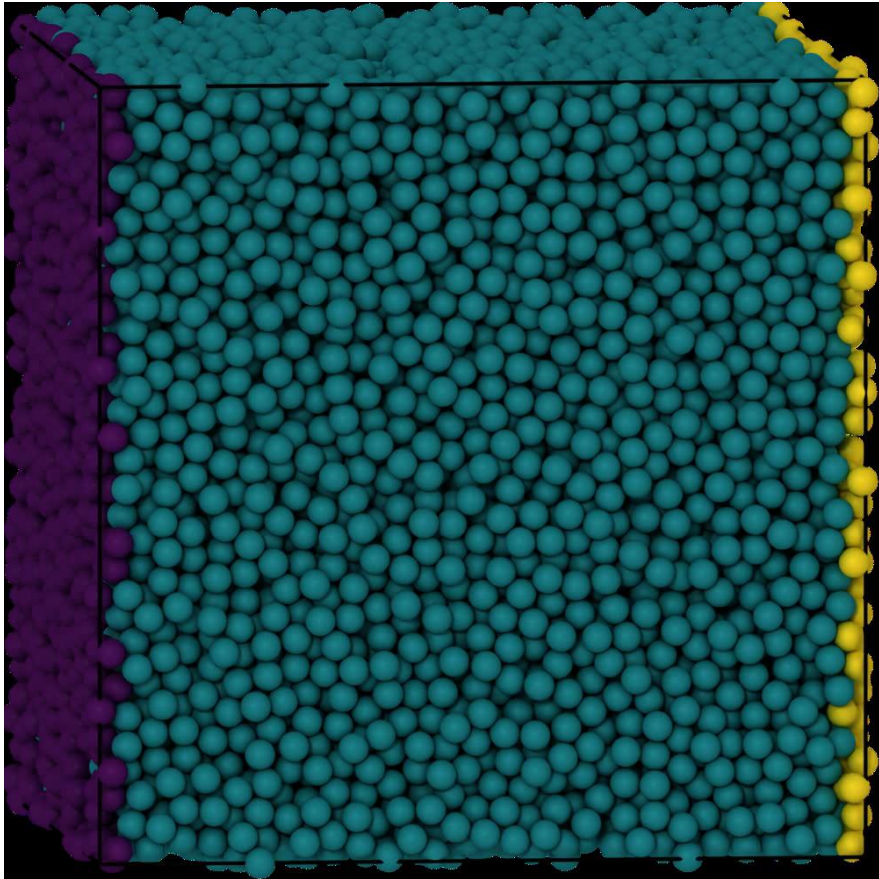


Visualization of a frequency oscillatory shear sweep (0.1 to 10 Hz) of bonded-particle resin matrix model.

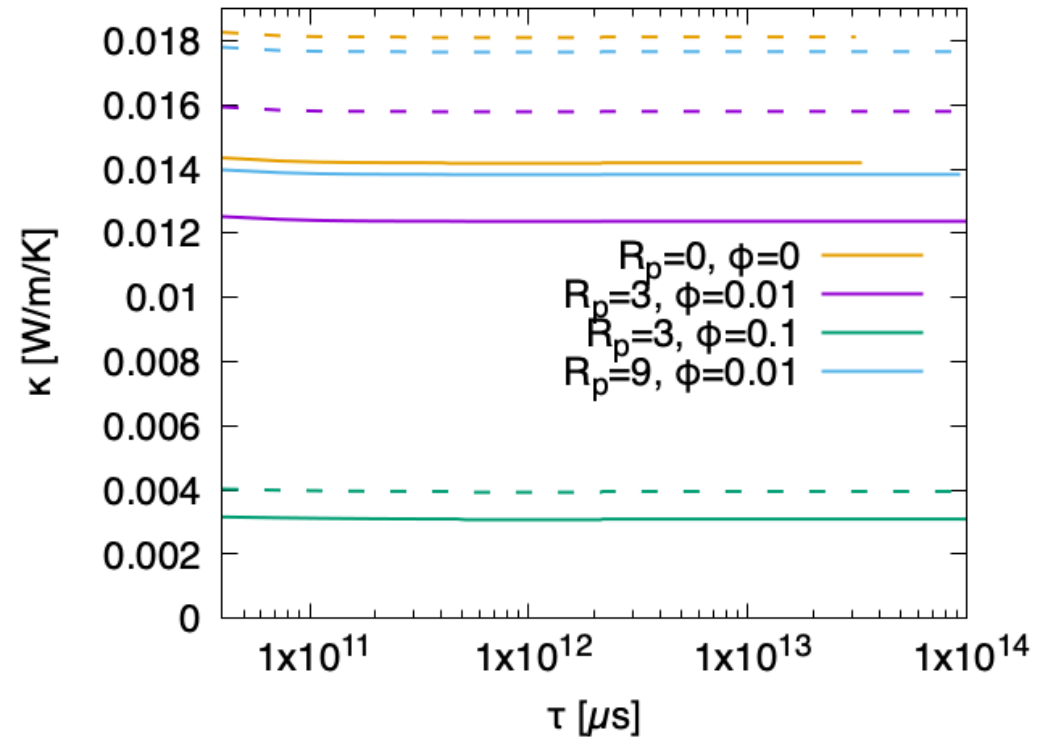


Simulation oscillatory shear stress (solid lines) wrt time for different pore structures. There is very little viscous damping, and thus near-zero loss modulus.

Thermal Conduction



Visualization of thermal gradient progression in phenolic.



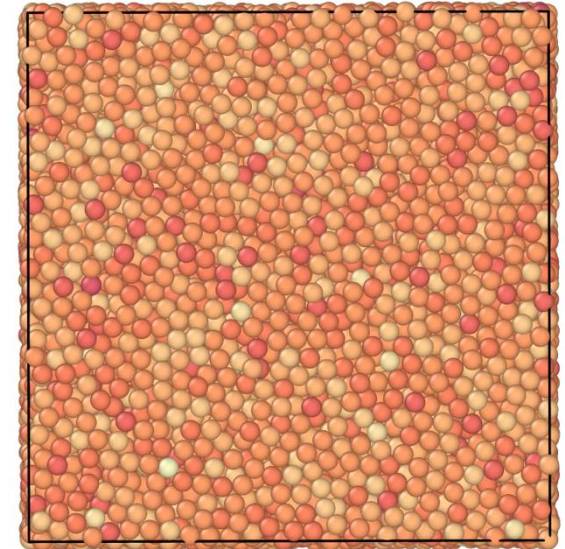
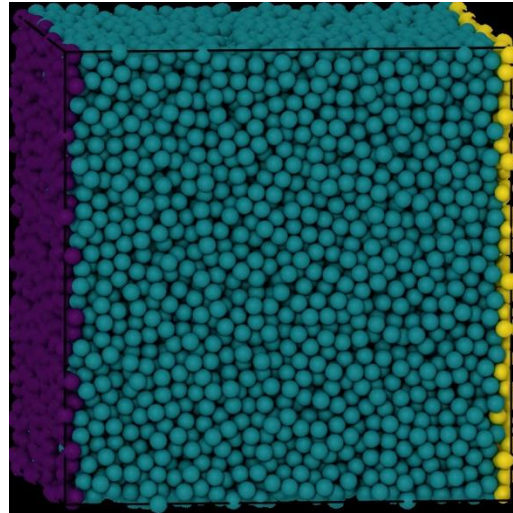
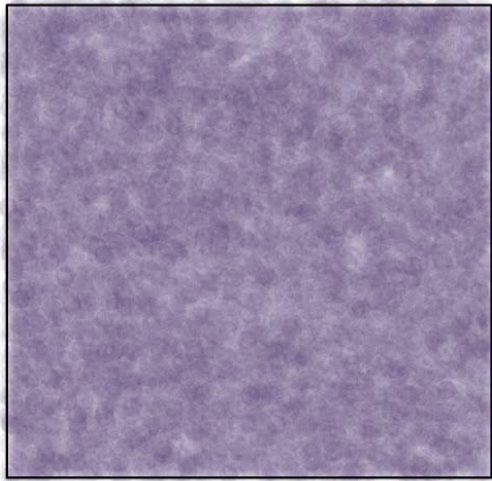
Preliminary conductivity vs time for $\langle N_{\text{bonds}} \rangle = 11$ (solid) and 1 (dashed), and porosity features.

Thank you, any questions?



Conclusions

- **Parameterized** bonded particle network model of phenolic
- Studied the role of random network **connectivity and porosity**



Next Steps

- Study **infused weaves** and networks
- **Verify** network behavior
- **In-situ** properties of phenolic in composites